



Meso-scale modeling of chloride diffusion in concrete with consideration of effects of time and temperature

Li-cheng WANG*¹, Tamon UEDA²

1. State Key Laboratory of Coastal and Offshore Engineering, Dalian University of Technology, Dalian 116024, P. R. China

2. Division of Built Environment, Hokkaido University, Sapporo 060-8628, Japan

Abstract: A meso-scale truss network model was developed to predict chloride diffusion in concrete. The model regards concrete as a three-phase composite of mortar matrix, coarse aggregates, and the interfacial transition zone (ITZ) between the mortar matrix and the aggregates. The diffusion coefficient of chloride in the mortar and the ITZ can be analytically determined with only the water-to-cement ratio and volume fraction of fine aggregates. Fick's second law of diffusion was used as the governing equation for chloride diffusion in a homogenous medium (e.g., mortar); it was discretized and applied to the truss network model. The solution procedure of the truss network model based on the diffusion law and the meso-scale composite structure of concrete is outlined. Additionally, the dependence of the diffusion coefficient of chloride in the mortar and the ITZ on exposure duration and temperature is taken into account to illustrate their effect on chloride diffusion coefficient. The numerical results show that the exposure duration and environmental temperature play important roles in the diffusion rate of chloride ions in concrete. It is also concluded that the meso-scale truss network model can be applied to chloride transport analysis of damaged (or cracked) concrete.

Key words: meso-scale modeling; concrete; chloride diffusion; truss network model

1 Introduction

Chloride-induced corrosion of reinforcing steel is one of the major causes of deterioration of reinforced concrete structures exposed to seawater or de-icing salt, such as marine structures and bridges. For the purpose of predicting the durability and service life of these structures, it is therefore very important to investigate the characteristics of chloride transport in concrete. Although the diffusivity problems of chloride have been examined in previous studies (Caré 2003), diffusivity has been difficult to estimate accurately because it depends on many factors, including the properties of the interfacial zone between aggregate particles and bulk cement pastes, and the microstructure of the cement paste itself (porosity and pore structure) (Oh and Jang 2004). As a result, the numerical simulation method has been applied

This work was supported by the Key Project of the Chinese Ministry of Education (Grant No. 109046), the Center for Concrete Core, Korea of the Yonsei University of Korea, and the Grant-in-Aid for Scientific Research from the Japanese Government (A) (Grant No. 19206048).

*Corresponding author (e-mail: wanglicheng2000@163.com)

Received Jul. 2, 2009; accepted Aug. 23, 2009

to analyze the transport of chloride ions in concrete with the purpose of understanding more of the factors. Besides the complex structure of concrete itself, many studies have found that the diffusion coefficient of chloride in concrete is dependent on environmental conditions such as the duration of exposure of structural members and the surrounding temperature (Nokken et al. 2006; Mangat and Molloy 1994; Xi and Bazant 1999). Most of these conclusions are based on experimental results. A numerical method that can consider the microstructure of concrete as well as the exposure circumstances would be a highly useful tool.

There are three levels of numerical simulation of concrete material: the macro-scale, meso-scale and micro-scale (Zhou and Hao 2008). At the macro-scale, concrete is treated as a homogeneous material. At the meso-scale, however, concrete is considered a composite of coarse aggregates, mortar matrix containing fine aggregates, and the ITZ. The ITZ is a zone in the vicinity of the aggregate particles in concrete that forms due to the water-filled pores near the aggregates and the wall effect. The microstructure of the ITZ differs significantly from that of the bulk cement paste (Delagrave et al. 1997; Shane et al. 2000). The ITZ's thickness is usually reported to be in the range of 15-50 μm , or less than 80 μm when the aggregate size varies from 0 to 20 mm (Otsuki et al. 2006). Typical values are around 20 μm (Bentz et al. 1995). If the mortar matrix of the meso-scale is subdivided into fine aggregate and hardened cement paste, the simulation becomes a micro-scale one. Of the three levels of analysis, meso-scale modeling is regarded as the most practical and useful method for evaluating the composite behavior of concrete. As a result, many meso-scale models have been developed to simulate the mechanical performance of concrete (Zhou and Hao 2008). However, little work has been done to use the meso-scale models to investigate the transport properties of concrete, especially to study the effects of exposure duration and temperature.

Experiments have shown that the diffusion coefficient of chloride in concrete is greatly dependent on the duration of exposure and the environmental temperature. This can be attributed to the effects of these parameters on the inner porosity and pore structure of concrete, since the hydration of cement paste continues over time and the temperature influences the movement of ions in the porous media of the concrete. Therefore, it is necessary to take the time and temperature effects into account in long-term durability analysis. However, the aggregates that are generally used, limestone and granite, are non-permeable, which implies that the permeability of aggregates themselves can be neglected and the time and temperature have no effect on them. According to experimental and numerical studies, the ITZ plays a very important role in a concrete mixture and it is a zone of weakness in the microstructure of concrete in terms of transport and mechanical properties (Delagrave et al. 1997; Takewaka et al. 2003; Yang 2003; Oh and Jang 2004). It is evident that the transport properties of the ITZ are influenced by environmental conditions. In other words, it would be more practical to treat concrete as a heterogeneous material and to consider the environmental factors separately, according to the intrinsic transport properties of concrete components.

The potential of meso-scale modeling in simulating the effects of loading on diffusion coefficient of chloride in concrete structures has been shown (Soda 2006; Wang et al. 2008). The objectives of this study were to use the meso-scale modeling method to predict the diffusion coefficient of chloride in concrete and to study the effects of different factors on the diffusion coefficient of chloride.

2 Governing equation for chloride diffusion

2.1 Basic equation

Fick's second law is usually used to describe chloride penetration by diffusion in saturated concrete. It can be represented by the following equation:

$$\frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2} \quad (1)$$

where D is the diffusion coefficient of chloride, and it is a constant here; and $C(x, t)$ is the chloride concentration at depth x from the exposed surface and time t . For a homogenous semi-infinite medium, the solution of Fick's second law is written as

$$C(x,t) = C_s - (C_s - C_0) \operatorname{erf} \left(\frac{x}{2\sqrt{Dt}} \right) \quad (2)$$

where C_s is the surface chloride concentration, C_0 is the initial chloride concentration, and erf is the standard error function. Although the movement of chloride in concrete is not a pure diffusion process from the point of view of mass transport, Eqs. (1) and (2) are still used due to their computational convenience.

As stated previously, concrete is not a homogenous material, but a multi-phase composite. Moreover, in most cases, cracks or micro-cracks occur in concrete due to shrinkage, thermal gradients, freeze-thaw cycling, alkali-aggregate reaction, external loads, or some combination of these causes. Hence, the diffusion of chloride in concrete is too complicated to be described with a single diffusion coefficient, although in some studies the apparent diffusion coefficient of chloride in concrete D_a is determined by fitting profiles of acid-soluble chloride concentration (obtained experimentally) versus depth with Eq. (2). Numerical analysis that investigates and quantifies the diffusion coefficient of chloride in each component of concrete is therefore a promising method for estimating the chloride diffusion coefficient in concrete, because each component can be treated as a relatively homogeneous material.

2.2 Analytical method of determining chloride diffusion coefficient in cement paste

A few models of the effective chloride diffusion coefficient in cement paste have been developed based on the assumption that cement paste is a two-phase composite of capillary pores and solid particles. Oh and Jang (2004) proposed an analytical model to predict the chloride diffusion coefficient in cement paste based on the capillary porosity, with the merit

that the model covers the entire capillary porosity range. The model can be expressed as

$$\frac{D_p}{D_0} = \left[m_\phi + \sqrt{m_\phi^2 + \frac{\phi_c}{1-\phi_c} \left(\frac{D_s}{D_0} \right)^{\frac{1}{n}}} \right]^n \quad (3)$$

where D_p is the effective chloride diffusion coefficient in cement paste; D_0 and D_s are, respectively, the chloride diffusion coefficient in the solid phase and the chloride diffusion coefficient in a continuum, e.g., ionic diffusion coefficient in bulk water; ϕ_c is the critical porosity of the pore network; and n is a constant called the percolation exponent. In this equation, m_ϕ is defined as

$$m_\phi = \frac{1}{2} \left\{ \left(\frac{D_s}{D_0} \right)^{\frac{1}{n}} + \frac{\phi_{\text{cap}}}{1-\phi_c} \left[1 - \left(\frac{D_s}{D_0} \right)^{\frac{1}{n}} \right] - \frac{\phi_c}{1-\phi_c} \right\} \quad (4)$$

where ϕ_{cap} is the capillary porosity.

n and D_s/D_0 values obtained from the test data are $n = 2.7$ and $D_s/D_0 = 2.0 \times 10^{-4}$ for Portland cement pastes (Oh and Jang 2004). In addition, the critical porosity ϕ_c is assumed to be 0.18 (Bentz and Garboczi 1991), which means that, when $\phi_c > 0.18$, the porosity controls the diffusion and the effect of the gel pores can be ignored. D_0 is assumed to be 2.032×10^{-9} m²/s at 25°C for chloride ions.

The capillary porosity, ϕ_{cap} , is estimated with the following equation (Hansen 1986):

$$\phi_{\text{cap}} = \frac{w/c - 0.36\alpha}{w/c + 0.32} \quad (5)$$

where w/c is the water-to-cement ratio, and α is the ultimate degree of hydration, defined as the weight fraction of the original cement, which has become hydrated. The capillary porosity predicted by Eq. (5) is a little higher than that proposed by Bentz and Garboczi (1991), which is expressed as follows:

$$\phi_{\text{cap}} = \frac{w/c - 0.41\alpha}{w/c + 0.313} \quad (6)$$

Eq. (5) was used in this study, since it is based on the classical Powers model (Hansen 1986). α is empirically expressed as a function of w/c (Oh and Jang 2004):

$$\alpha = 1 - \exp(-3.15w/c) \quad (7)$$

2.3 Chloride diffusion coefficient in mortar and ITZ

The inclusion of aggregates in a hydrated cement paste matrix usually has two opposite effects on the transport properties (Delagrave et al. 1997). On one hand, the addition of aggregate particles can increase the tortuosity of the matrix. As a result, the chloride ions have to move around the particles, which decreases the transport speed. On the other hand, the formation of the ITZ, which has a higher porosity and connectivity, probably facilitates greater mobility of ions. Therefore, in order to investigate the effect of aggregate content and the ITZ

on transport properties, the mortar can also be regarded as a three-phase composite material.

The chloride diffusion coefficient in the mortar has been described as follows (Oh and Jang 2004):

$$\frac{D_m}{D_p} = 1 + \frac{V_a}{\frac{1}{2D_{ITZ}/D_p \varepsilon - 1} + \frac{1 - V_a}{3}} \quad (8)$$

where D_m and D_{ITZ} are the chloride diffusion coefficients in the mortar and the ITZ, respectively; V_a is the volume fraction of aggregate particles; and ε is the ratio of the thickness of the ITZ to the radius of an aggregate particle, which may be approximated by considering the mean radius of aggregate particles. D_{ITZ} can also be estimated with Eq. (3), assuming that $\phi_{ITZ} = 1.5\phi_{cap}$. From this analysis, one can see that w/c is the dominant factor in the chloride diffusion coefficient in the mortar because of its crucial importance to the capillary porosity of cement paste (Sahu et al. 2004). Fig. 1 shows the effect of w/c on the D_m with various volume fractions of aggregate particles. D_m increases with w/c , due to the increase of the capillary porosity of the cement paste. The inclusion of aggregate particles can somewhat reduce the chloride diffusion coefficient, which indicates that, for mortar, the effect of tortuosity induced by aggregates is greater than that of the porosity and connectivity of the ITZ. Results from some experiments on the chloride diffusion coefficient in the mortar are also depicted in Fig. 1 to verify Eq. (8). Although the mixtures in those experiments were quite different from one another, the model represented by Eq. (8) shows a relatively good correlation with experimental data.

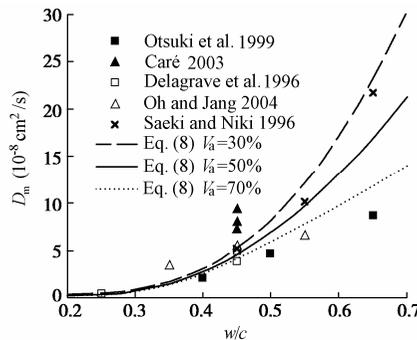


Fig. 1 Effects of w/c and V_a on D_m

2.4 Dependence of chloride diffusion coefficient on time and temperature

It is generally known that the chloride diffusion coefficient in mortar or concrete is time-dependent, as a result of the continuing hydration of the cement paste and the alteration of the capillary pore system. It is also temperature-dependent, due to its influence on the adsorption heat and the frequency of thermal vibration of the diffusant (Mangat and Molloy 1994; Xi and Bazant 1999). The following relationship has been proposed to account for the

influences of time and temperature on the chloride diffusion coefficient in concrete (Boddy et al. 1999):

$$D(t, T) = D_{\text{ref}} \left(\frac{t_{\text{ref}}}{t} \right)^n \exp \left[\frac{U}{R} \left(\frac{1}{T_{\text{ref}}} - \frac{1}{T} \right) \right] \quad (9)$$

where $D(t, T)$ is the diffusion coefficient of chloride at time t (d) and temperature T (K); D_{ref} is the diffusion coefficient of chloride at the reference time t_{ref} (d) and temperature T_{ref} (K), for mortar, which can be determined by Eqs. (3) and (8); n is a constant depending on mixture proportions, usually set at 0.2-0.3 for normal Portland cement mixtures, although its value is to some extent dependent on the experimental method (Nokken et al. 2006); U is the activation energy of the diffusion process (KJ/mol), which depends on the porosity and the cement type (values of U were provided by Xi and Bazant (1999)); and R is the gas constant (8.314 J/(mol·K)). The effects of time and temperature on the chloride diffusion coefficient are depicted in Fig. 2. The chloride diffusion coefficient shows a strong dependence on the time of the materials. On one hand, the chloride diffusion coefficient decreases with time, but the rate of descent gradually slows down. On the other hand, the chloride diffusion coefficient is quite sensitive to the temperature, and it increases along with the environmental temperature. Therefore, for structures in hot regions, adoption of the chloride diffusion coefficient values obtained from experimental study at normal temperatures will overestimate the service life. In order to obtain a more accurate long-term prediction of chloride diffusion coefficient in concrete, it is necessary that the analysis procedure take the time and temperature effects into account.

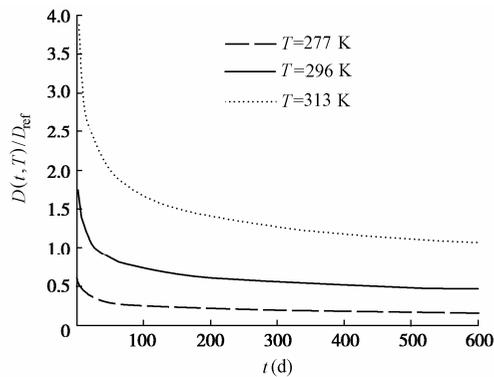


Fig. 2 Effects of time and temperature on diffusion coefficient of chloride ($t_{\text{ref}} = 28$ d and $T_{\text{ref}} = 296$ K)

3 Truss network model

3.1 Construction of truss network model

In this study, the Voronoi diagram was used as the meshing tool for the concrete specimen due to its advantages in simulating crack formation and propagation, as well as crack width, which are needed for predicting the deterioration and durability of concrete structures (Nagai

et al. 2004; Nakamura et al. 2006). The random geometrical characteristics of elements meshed using Voronoi diagrams make it possible to avoid prescribing the locations and directions of crack propagation because cracks initiate and propagate along the element boundaries. This means that adaptive re-meshing is not needed (Bolander and Le 1999). Fig. 3 shows the Voronoi diagram after meso-scale meshing of a concrete specimen.

The truss network model was based on the Voronoi diagram as shown in Fig. 3. The truss network was formed by linking nodes i at the centers of Voronoi elements with intermediate points j at Voronoi element boundaries mn (Fig. 4). This is a refined version of the approach proposed by Bolander and Berton (2004), which only linked the Voronoi nuclei to form a truss element. The truss elements and chloride diffusion in this study are consequently more realistic (Wang et al. 2008). It was assumed that the transport of substances (e.g., water or chloride ions) occurred along one-dimensional truss elements in the network. For concrete without cracks, the cross-sectional area and diffusion coefficient of truss elements in different phases of concrete were set according to the following rules: for truss elements in aggregates, both were assumed to be 0; for truss elements in mortars, the cross-sectional areas accorded with the corresponding Voronoi element area, explained below, and the diffusion coefficient was estimated with the method proposed in Section 2.3. At the Voronoi element boundaries, there were two kinds of truss elements. The first kind was at the interfaces of two mortar Voronoi elements, and its cross-sectional area was assumed to be 0 with no mass transfer occurrence. The second kind was just between the aggregates and mortars, i.e., the ITZ. Its cross-sectional area and diffusion coefficient were studied and determined through experiments and numerical analysis.

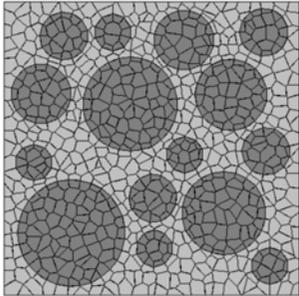


Fig. 3 Element geometry generated by Voronoi meshing

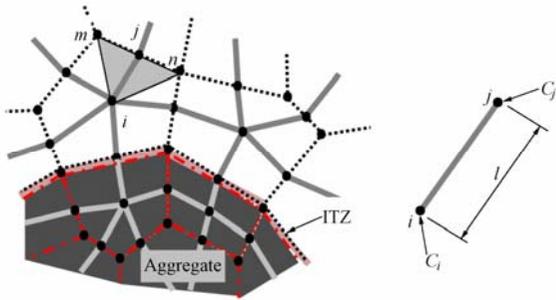


Fig. 4 Truss network model

3.2 Spatial discretization of governing equation

As shown in Fig. 4, in the truss network model, a continuous area is represented by the discrete truss network. Each kind of truss element has its own cross-sectional area and diffusion coefficient. For example, the diffusion area of Δ_{min} is represented by a one-dimensional truss element ij with a length of l (Fig. 4). In other words, the ions penetrating the area of Δ_{min} are mathematically considered along the one-dimensional truss

element ij . In this study, the weighted residual Galerkin method was used to discretize the nonlinear Eq. (1) numerically so that it could be easily applied to the truss network model.

For a one-dimensional finite element of length l , if the values of chloride concentration at the two end points i and j are respectively assumed to be C_i and C_j . The approximate expression of chloride concentration C at coordinate z along element ij can be linearly described as

$$C = \frac{z_j - z}{l} C_i + \frac{z - z_i}{l} C_j \quad (10)$$

where z_i and z_j are, respectively, the coordinate values of points i and j . For the sake of simplicity, one can set $g_i = \frac{z_j - z}{l}$ and $g_j = \frac{z - z_i}{l}$. These are regarded as the weighted residual functions. The following two error functions can be obtained with the Galerkin method:

$$\tilde{R}_i = A \int_{z_i}^{z_j} g_i \left(\frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial t} \right) dz = 0 \quad (11)$$

$$\tilde{R}_j = A \int_{z_i}^{z_j} g_j \left(\frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial t} \right) dz = 0 \quad (12)$$

where A is the cross-sectional area of the one-dimensional element. Soda (2006) described the integration process of error functions Eqs. (11) and (12). The final result is formulated as

$$\begin{bmatrix} +DA \frac{\partial C}{\partial z} \Big|_{z=z_i} \\ -DA \frac{\partial C}{\partial z} \Big|_{z=z_j} \end{bmatrix} + \frac{DA}{l} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} C_i \\ C_j \end{bmatrix} + \frac{1}{\omega} \frac{1A}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} \frac{\partial C_i}{\partial t} \\ \frac{\partial C_j}{\partial t} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (13)$$

where ω is a parameter that accounts for the dimension conversion, set at 2.0 for a two-dimensional truss element arrangement (Nakamura et al. 2006); and D can be a constant diffusion coefficient of chloride as given in Eq. (1) or a time- and temperature-dependent diffusion coefficient of chloride as shown in Eq. (9).

If only the diffusion process is considered when the chloride ions penetrate concrete, the initial condition and boundary condition below are applied to solve the difference equation described above:

$$\begin{cases} C = C_0, & z \geq 0, & t = 0 \\ C = C_s, & z = 0, & t > 0 \end{cases} \quad (14)$$

Then, Eq. (13) can be simplified:

$$\mathbf{f} + \mathbf{k}\mathbf{g} + \mathbf{p} \frac{\partial \mathbf{g}}{\partial t} = 0 \quad (15)$$

where $\mathbf{f} = \begin{bmatrix} +DA \frac{\partial C}{\partial x} \Big|_{z=z_i} \\ -DA \frac{\partial C}{\partial x} \Big|_{z=z_j} \end{bmatrix}$, $\mathbf{k} = \frac{DA}{l} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$, $\mathbf{g} = \begin{bmatrix} C_i \\ C_j \end{bmatrix}$, and $\mathbf{p} = \frac{1}{\omega} \frac{1A}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$. Eq. (13) is

the finite element equation for a single truss element. If all the truss elements in a meshed area are integrated, the global finite element equation is as follows:

$$\mathbf{F} + \mathbf{K}\mathbf{G} + \mathbf{P}\frac{\partial\mathbf{G}}{\partial t} = 0 \quad (16)$$

where \mathbf{F} , \mathbf{K} , \mathbf{G} , \mathbf{P} are, respectively, the items for the integrated all the truss elements corresponding to f , k , g , p . In this study, the Crank-Nicholson method was used to numerically solve the above equation. By introducing the discrete time step Δt , one obtains:

$$\mathbf{G}\left(t + \frac{\Delta t}{2}\right) = \frac{1}{2}[\mathbf{G}(t + \Delta t) + \mathbf{G}(t)] \quad (17)$$

Then, the difference formation at time $(t + \Delta t/2)$ in space-time can be expressed as

$$\frac{\partial}{\partial t}\mathbf{G}\left(t + \frac{\Delta t}{2}\right) = \frac{\mathbf{G}(t + \Delta t) - \mathbf{G}(t)}{\Delta t} \quad (18)$$

By substituting Eqs. (17) and (18) into Eq. (16), one can obtain:

$$\mathbf{F} + \frac{1}{2}\mathbf{K}[\mathbf{G}(t + \Delta t) + \mathbf{G}(t)] + \mathbf{P}\frac{1}{\Delta t}[\mathbf{G}(t + \Delta t) - \mathbf{G}(t)] = 0 \quad (19)$$

This yields the basic formulation for the discrete time calculation process:

$$\left(\frac{1}{2}\mathbf{K} + \frac{1}{\Delta t}\mathbf{P}\right)\mathbf{G}(t + \Delta t) = \left(-\frac{1}{2}\mathbf{K} + \frac{1}{\Delta t}\mathbf{P}\right)\mathbf{G}(t) - \mathbf{F} \quad (20)$$

Thus, with a step-by-step procedure, the chloride concentration profile in concrete at a given time, $C(x, t)$, can be calculated.

4 Results and discussion

4.1 Analysis conditions

Fig. 5 shows the geometry, boundary conditions and Voronoi diagram of a concrete specimen. Only the left side of the specimen was exposed to the chloride source, so that it could be regarded as the boundary. At the diffusion boundary, the chloride concentration was assumed to be $4.86 \times 10^{-3} \text{ g/cm}^3$. Chloride concentration was measured in grams of chloride per cm^3 of concrete (Saeki and Niki 1996). This value was calculated according to the capillary porosity of concrete and the chloride concentration in the exposed solution. If the density of concrete was considered to be 2.3 g/cm^3 , it would become $2.11 \times 10^{-3} \text{ g/g}$. The w/c was 0.55 and the volume content of coarse aggregates was about 40%, which implied that the sand volume fraction was about 50% for the mortar

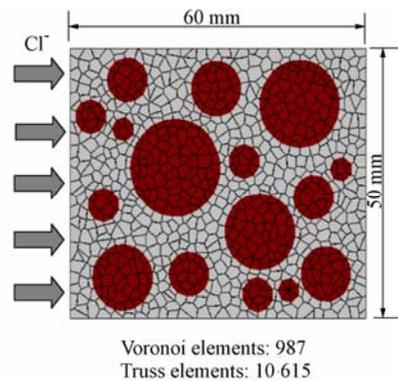


Fig. 5 Analysis conditions and Voronoi diagram of specimen

mixed in the concrete. In addition, based on our previous analysis, the chloride diffusion coefficient in the ITZ was determined to be 8.9 times that in the mortar with an ITZ thickness of 20 μm , which accords with some experimental results (Wang et al. 2008). In this study, therefore, the chloride diffusion coefficient in the ITZ was set at 9.0 times that in the mortar and the thickness of the ITZ was set at 20 μm .

4.2 Effect of time

The diffusion coefficient of chloride in the mortar is supposed to follow the law of time and temperature represented by Eq. (9), which is incorporated into the truss network model by substituting the constant diffusion coefficient D in Eq. (1) with the time-dependent expression of Eq. (9). For the purpose of demonstrating the influence of time on the diffusion coefficient of chloride, the temperature in Eq. (9) was assumed to be constant at 23°C, the general laboratory temperature. The effect of the time dependence of the chloride diffusion coefficient on the concentration profile of chloride in the truss network model simulation is shown in Fig. 6, with a reference time $t_{\text{ref}} = 28$ d, an exposure duration of 2000 d, and a discrete time step $\Delta t = 0.05$ d. If the reference time is 28 d, the chloride diffusion rate is quite slower than it is in the case in which the time effect is not considered. Fig. 7 shows the experimental profile of chloride concentration obtained by Mangat and Molloy (1994) in the case that $w/c = 0.40$, as well as the computational results when the chloride diffusion coefficient is the value at 28 days; it demonstrates a similar influential tendency of time to that in Fig. 6. However, it should be re-stated that the relative position of the two curves in Fig. 6 may shift if the reference time is greatly extended. The reason is that the diffusion coefficient $D(t, T)$ from Eq. (9) is always larger than D_{ref} before t_{ref} , but smaller than D_{ref} after t_{ref} . Consequently, if the diffusion coefficient is measured at an earlier time (e.g., 25 d), it will yield a larger value and result in a higher transport rate and subsequently conservative durability prediction; if the diffusion coefficient is measured after a longer time (e.g., 500 d), the predicted durability will be overestimated. The importance of the time effect is apparent from the above analysis.

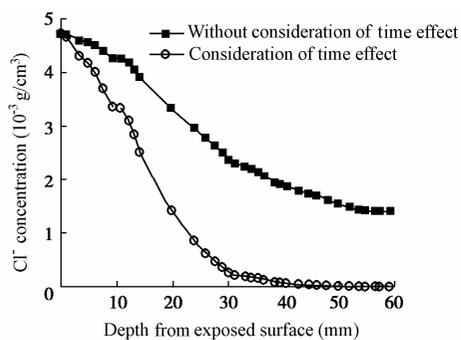


Fig. 6 Effect of time dependence of chloride diffusion coefficient on chloride concentration

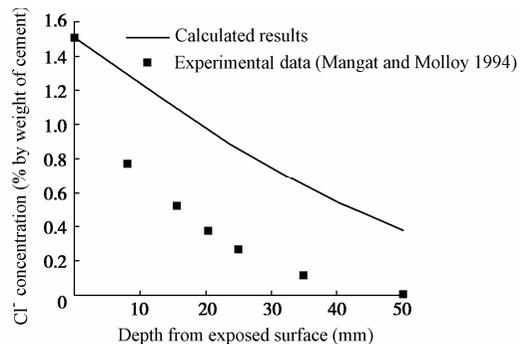


Fig. 7 Comparison of experimental data and analysis results without consideration of time effect

In the past few decades, service life prediction has become a common tool for performance-based specifications of concrete structures. Currently, the service life of a reinforced concrete structure is approximately estimated by assuming that the chloride concentration on the reinforcement surface reaches a threshold value. This study predicted chloride concentration profiles at a depth of 20 mm varying with time, with and without consideration of the time dependence of the chloride diffusion coefficient. They are shown in Fig. 8. For illustrative purposes, the threshold chloride concentration for reinforcement in concrete is assumed to be $1.0 \times 10^{-3} \text{ g/cm}^3$, although it depends to some extent on the concrete mixture proportions and environmental conditions (Hussain et al. 1996). Further attempts to properly quantify this parameter would contribute to the accuracy of service life prediction. It can be easily observed from Fig. 8 that the corrosion initiation time is 205 days when the time dependence is not considered, and 1 210 days when the time dependence is taken into account. It should be pointed out that the depth of reinforcement here, 20 mm, is only used to illustrate the significant influence of time on service life prediction, since the thickness of concrete cover is typically higher in an aggressive environment.

4.3 Effect of temperature

The profiles of chloride concentration after 600 days of exposure at temperatures of 4°C 23°C and 40°C were calculated and are presented in Fig. 9. Considering that the diffusion coefficient of chloride in the mortar is also time-dependent, however, we set an exposure time of 600 days in order to reduce the computing time. It can be clearly seen in Fig. 9 that the temperature has an impact on the chloride concentration profile, and certainly on the service life of the concrete structure. For an actual concrete structure, however, estimation of temperature is quite complicated, since the surrounding temperature is not constant but varies significantly. Therefore, it is imperative to know the temperature variation of the environment in order to improve the accuracy of prediction.

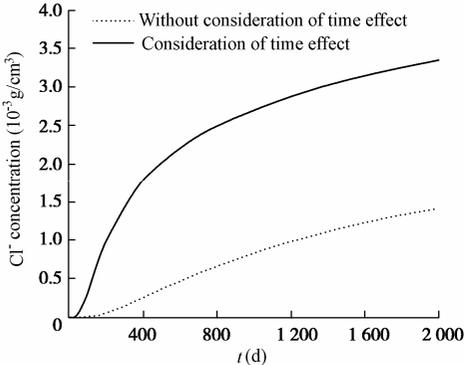


Fig. 8 Prediction of initiation time of reinforcement corrosion in two cases

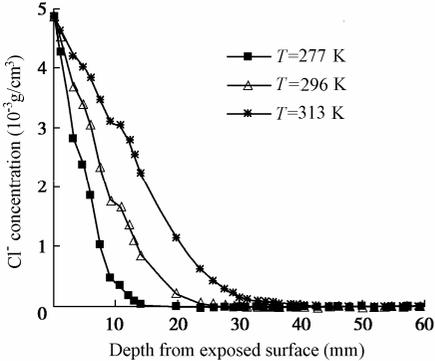


Fig. 9 Influence of temperature on chloride profile

5 Conclusions

A meso-scale truss network model was developed to simulate chloride diffusion in concrete, especially when the effects of time and temperature on diffusivity are taken into account. At the meso-scale, concrete was treated as a three-phase composite material, consisting of the coarse aggregates, the mortar matrix, and the ITZ. A method of analytically determining the diffusion coefficient of chloride in the mortar, mainly based on the water-to-cement ratio and the sand volume content when mortar itself is also assumed to be a multi-phase composite, was presented. Calculation results indicate that the truss network model can be used to efficiently predict the chloride diffusion coefficient in concrete by using only the mixture proportion and environmental conditions as input information. The significance of time was also illustrated by comparing the chloride concentration profiles obtained from two cases, one that considers the effect of time and one that does not. When the time dependence of the diffusion coefficient is not taken into account, the diffusion rate will be overestimated, on the contrary, it will be underestimated. The degree of influence depends on the selection of the reference time. Meanwhile, by comparing the concentration profiles of chloride at a series of constant temperatures, the temperature was also shown to have an important influence on the diffusion coefficient of chloride in concrete. However, it should be emphasized that, since the actual environmental temperature is variable, the monitoring of varying temperature on site over one year or throughout the service life of the structure helps to accurately predict the diffusion characteristics of chloride in concrete. This meso-scale simulation method can also be easily applied to the chloride transport analysis of damaged (or cracked) concrete, because cracks will accelerate the penetration of water and ions.

References

- Bentz, D. P., and Garboczi, E. J. 1991. Percolation of phases in a three-dimensional cement paste microstructural model. *Cement and Concrete Research*, 21(2-3), 325-344. [doi:10.1016/0008-8846(91)90014-9]
- Bentz, D. P., Detwiler, R. J., Garboczi, E. J., Halamickova, P., and Schwartz, L. M. 1995. Multi-scale modeling of the diffusivity of mortar and concrete. *Proceedings of Chloride Penetration into Concrete*, 85-94. Saint-Rémy-lès-Chevreuse: RILEM Publications.
- Boddy, A., Bentz, E., Thomas, M. D. A., and Hooton, R. D. 1999. An overview and sensitivity study of a multimechanistic chloride transport model. *Cement and Concrete Research*, 29(6), 827-837. [doi:10.1016/S0008-8846(99)00045-9]
- Bolander, J. E., and Le, B. D. 1999. Modeling crack development in reinforced concrete structures under service loading. *Construction Building Material*, 13(1-2), 23-31. [doi:10.1016/S0950-0618(99)00005-7]
- Bolander, J. E., and Berton, S. 2004. Simulation of shrinkage induced cracking in cement composite overlays. *Cement and Concrete Composites*, 26(7), 861-871. [doi:10.1016/j.cemconcomp.2003.04.001]
- Caré, S. 2003. Influence of aggregates on chloride diffusion coefficient into mortar. *Cement and Concrete Research*, 33(7), 1021-1028. [doi:10.1016/S0008-8846(03)00009-7]
- Delagrave, A., Marchand, J. and Samson, E. 1996. Prediction of diffusion coefficients in cement-based materials on the basis of migration experiments. *Cement and Concrete Research*, 26(12), 1831-1842.
- Delagrave, A., Bigas, J. P., Ollivier, J. P., Marchand, J., and Pigeon, M. 1997. Influence of the interfacial zone

- on the chloride diffusivity of mortars. *Advanced Cement Based Materials*, 5(3), 86-92. [doi:10.1016/S1065-7355(96)00008-9]
- Hansen, T. C. 1986. Physical structure of hardened cement paste: A classical approach. *Materials and Structures*, 9(114), 423-436. [doi:10.1007/BF02472146]
- Hussain, S. E., Al-Gahtani, A. S., and Rasheeduzzafar. 1996. Chloride threshold for corrosion of reinforcement in concrete. *ACI Material Journal*, 93(6), 1-5.
- Mangat, P. S., and Molloy, B. T. 1994. Prediction of long term chloride concentration in concrete. *Materials and Structures*, 27(6), 338-346. [doi:10.1007/BF02473426]
- Nagai, K., Sato, Y., and Ueda, T. 2004. Mesoscopic simulation of failure of mortar and concrete by 2D RBSM. *Journal of Advanced Concrete Technology*, 2(3), 359-374.
- Nakamura, H., Srisoros, W., Yashiro, R., and Kunieda, M. 2006. Time-dependent structural analysis considering mass transfer to evaluate deterioration process of RC structures. *Journal of Advanced Concrete Technology*, 4(1), 147-158.
- Nokken, M., Boddy, A., Hooton, R. D., and Thomas, M. D. A. 2006. Time dependent diffusion in concrete-three laboratory studies. *Cement and Concrete Research*, 36(1), 200-207. [doi:10.1016/j.cemconres.2004.03.030]
- Oh, B. H., and Jang, S. Y. 2004. Prediction of diffusivity of concrete based on simple analytic equations. *Cement and Concrete Research*, 34(3), 463-480. [doi:10.1016/j.cemconres.2003.08.026]
- Otsuki, N., Hisada, M., Otani, T., and Maruyama, T. 1999. Theoretical evaluation of diffusion coefficient of chloride ion in mortar from mobility. *ACI Materials Journal*, 96(6), 627-633.
- Otsuki, N., Nishida, T., Wattanachai, P., and Chin, K. 2006. Experimental study on influence of ITZ around aggregate on Cl⁻ diffusivity of concrete. *Journal of the Society Material Science*, 55(10), 899-904. (in Japanese)
- Saeki, T., and Niki, H. 1996. Migration of chloride ions in non-saturated mortar. *Proceeding of Japan Concrete Institute*, 18(1), 969-974. (in Japanese)
- Sahu, S., Badger, S., Thaulow, N., and Lee, R. J. 2004. Determination of water-cement ratio of hardened concrete by scanning electron microscopy. *Cement and Concrete Composite*, 16(8), 987-992. [doi:10.1016/j.cemconcomp.2004.02.032]
- Shane, J. D., Mason, T. O., and Jennings, H. M. 2000. Effect of the interfacial transition zone on the conductivity of Portland cement mortars. *Journal of the American Ceramic Society*, 83(5), 1137-1144.
- Soda, M. 2006. *Chloride Diffusion Analysis for Cracked Concrete by RBSM*. M. E. Dissertation. Sapporo: Hokkaido University.
- Takewaka, K., Yamaguchi, T., and Maeda, S. 2003. Simulation model for deterioration of concrete structures due to chloride attack. *Journal of Advanced Concrete Technology*, 1(2), 139-146.
- Wang, L., Soda, M., and Ueda, T. 2008. Simulation of chloride diffusivity for cracked concrete based on RBSM and truss network model. *Journal of Advanced Concrete Technology*, 6(1), 143-155.
- Xi, Y. P., and Bazant, Z. P. 1999. Modeling chloride penetration in saturated concrete. *Journal of Materials in Civil Engineering*, 11(1), 58-65.
- Yang, C. C. 2003. Effect of the interfacial transition zone on the transport and the elastic properties of mortar. *Magazine of Concrete Research*, 55(4), 305-312. [doi:10.1680/macr.55.4.305.37586]
- Zhou, X. Q., and Hao, H. 2008. Mesoscale modelling of concrete tensile failure mechanism at high strain rates. *Computers and Structures*, 86(21-22), 2013-2026. [doi:10.1016/j.compstruc.2008.04.013]